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Electron dispersion in a three-dimensional regimented quantum dot superlattice

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Abstract. The electron band structure in a three-dimensional *regimented* quantum dot superlattice is analyzed using an envelope function approximation. It is shown that the electron density of states, effective mass, and carrier mobility in these structures are drastically different from those in quantum well superlattices and bulk materials. By changing the size of quantum dots, inter-dot distances, barrier height and regimentation, one can effectively tune the electronic properties of the quantum dot superlattices and make them suitable for a variety of device applications.

Introduction

Quantum dot arrays or stacks of quantum dot arrays, which we refer to as quantum dot superlattices (QDS), feature very different degrees of periodicity. Quantum dots grown by molecular beam epitaxy (MBE) can be completely random in such structures, partially regimented, like in QDS with vertical dot site correlation [1], or may have very high degree of regimentation [2]. Although many types of regimented QDS have been fabricated using different self-assembly techniques [3], very little attention has been paid to a theoretical description of electron spectrum in such structures [4].

The goal of this work is to develop a model for calculating the electronic structure in QDS that can serve as a useful tool for experimentalists and materials growers. To achieve this goal, we limit ourselves to the envelope function approximation and the perturbation theory. We show that our approach can provide the accuracy comparable to other treatments such as the finite-elements method, and plain-wave expansion technique. The regimentation, e.g. long-range spatial ordering, of quantum dots along all three directions results in the formation of an artificial crystal, where quantum dots play the role of atoms. Thus, this structure can also be referred to as a *quantum dot crystal* (QDC).

It is well known that the solution of Schrödinger equation in the three-dimensional space can be greatly simplified if the potential $V(x, y, z)$ is written as a sum of three independent potential functions of coordinates x, y, and z. We use this specific form of the confining potential as a zero approximation for our solution. Then we apply the time-independent perturbation theory in order to obtain a solution for the potential of interest, which is quantum dot potential well surrounded from each side by the barriers of equal height. A particular choice of the values of the zero-approximation and perturbing potentials allows us to make the corrections to our initial solution rather small. It is interesting to note that our initial choice of spatially separable potential corresponds to the real potential profile in quantum dots induced by strain from buried stressors [5].

For this work, the numerical simulations are carried out for a QDC that consists of very small (feature size is on the order of 5–10 nm) Ge quantum dots embedded in Si. This

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structure is similar to multiple arrays of Ge quantum dots grown on (001) Si by solid-source MBE [ ]. Approximately 90% of the band offset in such structure goes to the valence band. Due to this reason, our analysis is restricted to heavy holes in Ge/Si QDC. The light-hole states are split and located above the barrier due to the strain effects. The band offset for the heavy holes is approximately equal to 0.45 eV. In our calculations we used the following values for the effective masses $m^*_W = m^*_{\mathrm{Ge}} = 0.28m_0$ and $m^*_B = m^*_{\mathrm{Si}} = 0.49m_0$.

1. Electron dispersion

Figure 1 presents electron dispersion in a *simple cubic* QDC along the [[111]] *quasi*-crystallographic direction. Here the directions denoted with double square brackets are associated with the ordering of the quantum dots and are not related to the symmetry directions of the Si crystal itself. The energy bands are denoted by three quantum numbers $n_x n_y n_z$ with the superscript indicating the degeneracy of the band. The spin degeneracy is not counted here. Like in real crystals, the energy in QDC has the full symmetry of the reciprocal lattice. The energy bands are degenerated in the center of the *quasi*-Brillouin zone (QBZ) of the artificial crystal. The highest, sixfold, degeneracy is achieved in mini-bands of *cubic* QDC characterized by different quantum numbers $n_x n_y n_z$. If two of these three quantum numbers are equal, the degeneracy is threefold. Finally, if $n_x = n_y = n_z$

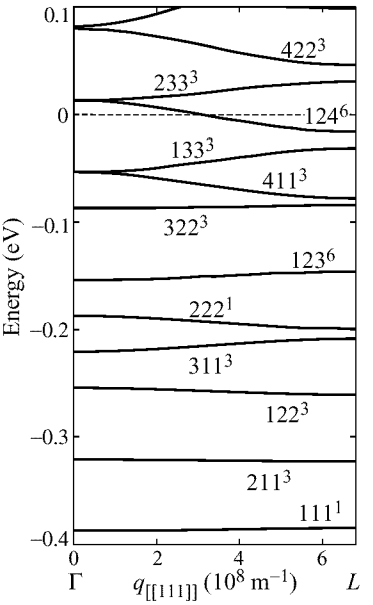

Fig. 1. Dispersion relation in a cubical quantum dot crystal shown along [[111]] quasi-crystallographic direction. The energy in units of eV is counted from the position of the potential barrier. The dot size is $L_x = L_y = L_z = 6.5$ nm and the inter-dot distance is $H_x = H_y = H_z = 1.5$ nm. Material parameters used in simulation correspond to the valence band of Ge/Si system.

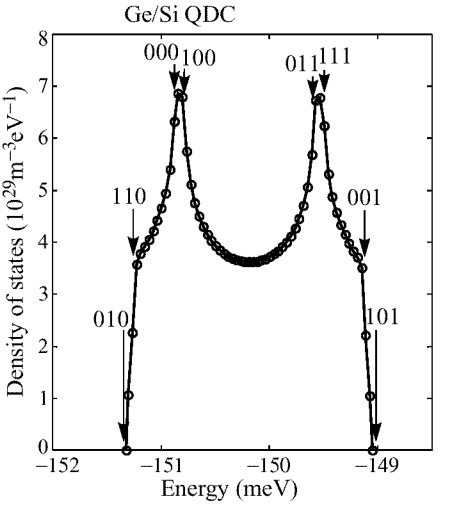

Fig. 2. Electron density of states in a cubical quantum dot crystal for 3D mini-bands defined by the following quantum numbers $n_x = 1, n_y = 2$, and $n_z = 3$. The dot size is $L_x = L_y = L_z = 6.5$ nm and the inter-dot distance is $H_x = H_y = H_z = 1.5$ nm. The arrows in this figure indicate particular quasi-crystallographic points. The energy in units of meV is counted from the position of the potential barrier.

there is no symmetry degeneracy in such a mini-band. Moving from the point of high symmetry in the center of the QBZ to a point of lower symmetry, the energy bands split. Unlike in real crystals, in artificial quantum dot crystal the degeneracy can be up to sixfold along [[111]] quasi-crystallographic direction even far from the center of QBZ. This is a result of the cubic symmetry both of the dot and the superlattice (see Fig. 1). If their symmetries are different, the twofold degeneracy will be the maximum permitted in all directions.

2. Density of states

An electron (hole) density of states (DOS) has been calculated taking into account the twofold electron spin degeneracy. The results of our numerical simulation of DOS in a cubic QDC for the most intricate case of all different quantum numbers $n_x = 1$, $n_y = 2$, and $n_z = 3$ are presented in Fig. 2. The points of high symmetry correspond to analytic critical points with van Hove singularities. The shape of DOS is defined by the quantum numbers of the corresponding mini-band. The arrows in this figure indicate particular quasi-crystallographic points. One should mention here that the areas under each DOS curve corresponded to different dispersion brunches, e.g. integral of each DOS, are all equal and defined by the density of quantum dots in a crystal. Note that the shape of DOS in the quantum dot crystal is drastically different from that in the quantum well superlattice and random quantum dot (QD) array.

3. Effective mass tensor and mobility of carriers

The simulation shows that the effective mass and the group velocity in QDC is highly anisotropic and strongly dependent on the mini-band index, e.g. quantum numbers which define the mini-band. The effective mass strongly depends on the periodicity and regimentation of the dots in the artificial crystal. It is almost always different from that one in the corresponding bulk material, and changes dramatically within a very narrow range of energy. This leads to a strong modification of the carrier mobility and conductivity in such structures.

The carrier motion perpendicular to the sides of quantum dots is completely defined by only one quantum number that describes quantization in the direction of motion. In this case a family of mini-bands is characterized by the same effective mass. Thus, along [[100]] direction, electron (hole) transport in QDC is similar to the one in conventional quantum well superlattices. The effective mass along [[110]] direction is determined by two quantum numbers, so that few mini-bands have the same value of the effective mass. Transport along [[111]] direction, e.g. cube diagonal, is more complicated and the effective mass is different for each branch. Application of electric field along this direction would initiate electron (hole) transport drastically different from that in quantum well superlattices.

4. Conclusion

The carrier band structure in a three-dimensional *regimented* quantum dot superlattice, e.g. quantum dot crystal, has been analyzed. Numerical simulations have been carried out for the valence band of a Ge/Si quantum dot crystals with the quantum dot feature size on the order of 5–10 nm. By changing the size of quantum dots, inter-dot distances, barrier height and regimentation, one can control the electronic properties of this artificial crystal, which are significantly different from those in bulk, quantum well superlattices, and random QD array.

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